

# Formulas for Rational-Valued Separability Probabilities of Random Induced Generalized Two-Qubit States

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## Abstract

Previously, a formula, incorporating a  ${}_5F_4$  hypergeometric function, for the Hilbert-Schmidt-averaged determinantal moments  $\langle |\rho^{PT}|^n |\rho|^k \rangle / \langle |\rho|^k \rangle$  of  $4 \times 4$  density-matrices ( $\rho$ ), and their partial transposes ( $\rho^{PT}$ ) was applied with  $k = 0$  to the generalized two-qubit separability-probability question. The formula can, further, be viewed we note here, as an averaging over “induced measures in the space of mixed quantum states”. The associated induced-measure separability probabilities ( $k = 1, 2, \dots$ ) are found—*via* a high-precision density approximation procedure—to assume interesting, relatively simple rational values in the two-re[al]bit ( $\alpha = \frac{1}{2}$ ), (standard) two-qubit ( $\alpha = 1$ ) and two-quater[nionic]bit ( $\alpha = 2$ ) cases. We deduce rather simple companion (rebit, qubit, quaterbit, ...) formulas that successfully reproduce the rational values assumed for *general*  $k$ . These formulas are observed to share certain features, possibly allowing them to be incorporated into a single master formula.

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## I. INTRODUCTION

The question of the probability that a generic quantum system is separable/disentangled was raised in a 1998 paper of Życzkowski, Sanpera, Lewenstein and Horodecki, entitled "Volume of the set of separable states" [1]. Certainly, any particular answer to this question will crucially depend upon the measure that is attached to the systems in question. A large body of literature has arisen from the 1998 study, and we seek to make a significant contribution to it, addressing heretofore unsolved problems. Let us point out the work of Aubrun, Szarek and Ye [2], which addresses questions of a somewhat similar nature to those examined below, while employing the same class of measures. However, their work is set in an *asymptotic* framework, while we will be concerned with obtaining exact *finite-dimensional* results (cf. [3]). On the other hand, Singh, Kunjwal and Simon [4] did focus on finite-dimensional scenarios, but with a distinct form of measure, the one originally used in [1].

We have investigated the possibility of extending to the class of "induced measures in the space of mixed quantum states" [5, 6] the line of analysis reported in [7, 8], the principal separability probability findings of which—most notably the two-qubit conjecture of  $\frac{8}{33} \approx 0.242424$ —have recently been robustly supported, with the use of extensive Monte-Carlo sampling, by Fei and Joynt [9], as well as by Milz and Strunz, to somewhat similar effect [10, Fig. 4, eqs. (30), (31)] (cf. [11, Table 1]). This earlier line of work pertained to the use of the Hilbert-Schmidt measure (the particular symmetric case,  $K = N$ , of the induced measures) on the high-dimensional convex sets of generalized (real-, complex-, quaternionic-entried) two-qubit ( $N = 4$ ) states.

In [7, p. 30], a central role had been played by the (not yet formally proven) determinantal moment formula obtained there

$$\begin{aligned} & \left\langle |\rho^{PT}|^n |\rho|^k \right\rangle / \left\langle |\rho|^k \right\rangle \\ &= \frac{(k+1)_n (k+1+\alpha)_n (k+1+2\alpha)_n}{2^{6n} (k+3\alpha+\frac{3}{2})_n (2k+6\alpha+\frac{5}{2})_{2n}} \\ & \cdot {}_5F_4 \left( \begin{matrix} -n, -k, \alpha, \alpha + \frac{1}{2}, -2k-2n-1-5\alpha \\ -k-n-\alpha, -k-n-2\alpha, -\frac{k+n}{2}, -\frac{k+n-1}{2} \end{matrix}; 1 \right) \end{aligned}$$

on the basis of extensive computations. Here  $\rho^{PT}$  denotes the partial transpose [12] of the density matrix  $\rho$ , and  $|\rho|$ , its determinant, and generalized hypergeometric function notation

is employed. The brackets represent averaging with respect to Hilbert-Schmidt measure [13]. Furthermore,  $\alpha$  is a random-matrix Dyson-index-like parameter [14], assuming, in particular, the value 1 for the standard (fifteen-dimensional convex set of) density matrices with complex-valued off-diagonal entries.

It subsequently occurred to us that this hypergeometric-based moment formula could be readily adapted to the broader class of random induced measures by considering, in the notation of [5, 6] that

$$k = K - N, \quad (1)$$

where  $K$  is the dimension of the ancilla/environment state, over which the tracing operation is performed.

As in the earlier work [7, 8], a high-precision density-approximation (inverse) procedure of Provost, incorporating the first 11,401 such determinantal moments, strongly indicates that the random induced-measure separability probabilities ( $k = 1, 2, \dots$ ) assume interesting, relatively simple rational values in the two-re[al]bit ( $\alpha = \frac{1}{2}$ ), (standard) two-qubit ( $\alpha = 1$ ) and two-quater[nionic]bit ( $\alpha = 2$ ) cases, particularly so for  $\alpha = 1$  (sec. II). One striking example is that for  $k = 3$ , the  $\alpha = 1$  separability probability is found to be  $\frac{27}{38} = \frac{3^3}{2 \cdot 19}$  (to *fifteen* decimal places). In fact, based on extensive calculations ( $k = 0, \dots, 15, \dots$ ) of this nature, we are able to deduce rather simple companion (rebit, qubit, quaterbit) formulas (2)-(4) that successfully reproduce the rational values assumed for *general* integer and half-integer  $k$  (sec. III).

Further efforts along these lines have been given in a subsequent paper [15], in which the determinantal inequality  $|\rho^{PT}| > |\rho|$  is now imposed, rather than the broader inequality  $|\rho^{PT}| > 0$ . (Of course,  $|\rho| \geq 0$ , while  $|\rho^{PT}|$  is both a necessary and sufficient condition for separability here [12, 16].) There, equivalent hypergeometric- and difference-equation-based formulas,  $Q(k, \alpha) = G_1^k(\alpha)G_2^k(\alpha)$ , for  $k = -1, 0, 1, \dots, 9$ , were given for that (rational-valued) portion of the total separability probability satisfying the stricter inequality. (We also preliminarily investigate this problem below in sec. IV.)

Milz and Strunz [10] have recently reported a highly interesting finding that the conjectured Hilbert-Schmidt separability probability of  $\frac{8}{33} \approx 0.242424$  holds constant along the radius of the Bloch sphere of either of the reduced subsystems of generic two-qubit ( $\alpha = 1$ ) systems. We are presently investigating the nature that the separability probability takes as a *joint* function of the radii of the two single-qubit subsystems, and related questions.

## II. ANALYSIS

We pursue the indicated extension of our earlier (Hilbert-Schmidt-based) work to random induced measures, in general. As in [7, 8], the determinantal moment formula above is employed in the Legendre-polynomial-based (Mathematica-implemented) density approximation (inverse) procedure of Provost [17]. This possesses a least-squares rationale. The program as originally presented is speeded, by incorporating the well-known recursion formula for Legendre polynomials, so that successive polynomials do not have to be computed *ab initio*. The computations are all exact, in nature, rather than numerical. Provost advises that the procedure should be regarded as an "approximation", rather than an "estimation" scheme [17]. (Let us note that the implementation of the procedure requires considerable caution and an adaptive strategy when the term  $(k-j+1)_{n-j}$  [7, sec. D.2] in the underlying summation formula for the hypergeometric-based determinantal moments is zero. It is zero if  $k-j+1 \leq 0 \leq k+n-2j$ , that is, if values  $j$  for which  $k+1 \leq j$  and  $2j \leq k+n$  occur in the summation  $j = 0 \dots n$ .)

Now, with the use of an unprecedentedly large number (11,401) of the determinantal moments, we found (to ten decimal places) for  $k = 1$ , the separability probability of the standard, complex ( $\alpha = 1$ ) 15-dimensional convex set of two-qubit states to be  $\frac{61}{143} = \frac{61}{11 \cdot 13} \approx 0.4265734$ . On the other hand, for the Hilbert-Schmidt case ( $k = K - N = 0$ ), a very compelling body of evidence of a number of types (though yet no formal proof) has been adduced that the corresponding separability probability, as has been already noted, is  $\frac{8}{33} = \frac{2^3}{3 \cdot 11} \approx 0.242424$  [7–10].

For the quaternionic ( $\alpha = 2$ ) case, the induced-measure ( $k = 1$ ) separability probability (now to thirteen decimal places) was  $\frac{3736}{22287} = \frac{2^3 \cdot 467}{3 \cdot 17 \cdot 19 \cdot 23} \approx 0.16763135$ , while the Hilbert-Schmidt counterpart strongly appears to be  $\frac{26}{323} = \frac{2 \cdot 13}{17 \cdot 19} \approx 0.0804953$  [7–9].

Let us further note, though any immediate quantum-mechanical random-matrix division-algebra interpretation does not seem at hand, that for  $k = 1, \alpha = 3$ , we obtain a "separability-probability" approximant, based on the 11,401 moments, that, to a remarkable *sixteen* decimal places equalled  $\frac{8159}{124062} = \frac{41 \cdot 199}{2 \cdot 3 \cdot 23 \cdot 29 \cdot 31} \approx 0.0657655$ . This particularly high accuracy appears to essentially be an artifact of the Legendre-polynomial-based procedure that commences with a *uniform* distribution over the the interval  $|\rho| \in [-\frac{1}{16}, \frac{1}{256}]$ . For such a distribution, the probability over the "separability" interval of  $[0, \frac{1}{256}]$  is the ratio of  $\frac{1}{256}$  to

TABLE I: Two-Rebit ( $\alpha = \frac{1}{2}$ ) Separability Probabilities

$k = 0$	$\frac{29}{64}$	$\frac{29}{2^6}$	0.453125
$k = 1$	$\frac{515}{768}$	$\frac{5 \cdot 103}{2^{8 \cdot 3}}$	0.670573
$k = 2$	$\frac{1645}{2048}$	$\frac{5 \cdot 7 \cdot 47}{2^{11}}$	0.803222
$k = 3$	$\frac{31641}{35840}$	$\frac{3 \cdot 53 \cdot 199}{2^{10 \cdot 5 \cdot 7}}$	0.882840
$k = 4$	$\frac{274373}{294912}$	$\frac{11 \cdot 24943}{2^{15 \cdot 3^2}}$	0.930355
$k = 5$	$\frac{439777}{458752}$	$\frac{13 \cdot 33829}{2^{16 \cdot 7}}$	0.958638
$k = 6$	$\frac{11251151}{11534336}$	$\frac{11251151}{2^{20 \cdot 11}}$	0.975448
$k = 7$	$\frac{30224045}{30670848}$	$\frac{5 \cdot 17 \cdot 53 \cdot 6709}{2^{18 \cdot 3^2 \cdot 13}}$	0.985432
$k = 8$	$\frac{10395147}{10485760}$	$\frac{3 \cdot 7 \cdot 19 \cdot 26053}{2^{21 \cdot 5}}$	0.991358

$(\frac{1}{16} + \frac{1}{256})$ , that is  $\frac{1}{17} \approx 0.0588235$ , quite near to 0.0657655. So as separability probability approximants increasingly deviate from the uniform-based one of  $\frac{1}{17}$ , at least for specific  $k$ , we can expect convergence of the density-approximation procedure to relatively weaken.

For the two-rebit scenario ( $\alpha = \frac{1}{2}$ ), the associated Hilbert-Schmidt separability probability strongly appears to be  $\frac{29}{64} = \frac{29}{2^6} \approx 0.453125$  [7, 8], while in the random induced-measure  $k = 1$  counterpart, we obtain (to almost nine decimal places) a value once again larger than that for the Hilbert-Schmidt case of  $k = 0$ , that is,  $\frac{515}{768} = \frac{5 \cdot 103}{2^{8 \cdot 3}} \approx 0.670573$ . (Note the powers of 2, in both denominators—a phenomenon that will continue to be observed for rebit-related results.)

In Tables I, II and III, we present our conclusions, based on such high-precision calculations, as to the rational values ( $k = 0, 1, \dots, 8$ ) assumed by these induced-measure separability probabilities. Let us note that with the sole exception of  $k = 7$ , the rational values assumed by the (standard) two-qubit ( $\alpha = 1$ ) induced states have both smaller denominators and numerators than the other two cases tabulated, indicative, presumably, in some manner, of their greater "naturalness".

### III. THREE COMPANION SEPARABILITY PROBABILITY FORMULAS

Further extending the entries of the two-qubit table (Table II), but not explicitly showing the results here, to  $k = 17$ , application of the Mathematica command FindSequenceFunc-

TABLE II: Two-Qubit ( $\alpha = 1$ ) Separability Probabilities

$k = 0$	$\frac{8}{33}$	$\frac{2^3}{3 \cdot 11}$	0.242424
$k = 1$	$\frac{61}{143}$	$\frac{61}{11 \cdot 13}$	0.426573
$k = 2$	$\frac{259}{442}$	$\frac{7 \cdot 37}{2 \cdot 13 \cdot 17}$	0.585973
$k = 3$	$\frac{27}{38}$	$\frac{3^3}{2 \cdot 19}$	0.710526
$k = 4$	$\frac{5960}{7429}$	$\frac{2^3 \cdot 5 \cdot 149}{17 \cdot 19 \cdot 23}$	0.802261
$k = 5$	$\frac{379}{437}$	$\frac{379}{19 \cdot 23}$	0.867277
$k = 6$	$\frac{63881}{70035}$	$\frac{127 \cdot 503}{3 \cdot 5 \cdot 7 \cdot 23 \cdot 29}$	0.912129
$k = 7$	$\frac{1169237}{1240620}$	$\frac{37 \cdot 31601}{2^2 \cdot 3 \cdot 5 \cdot 23 \cdot 29 \cdot 31}$	0.942461
$k = 8$	$\frac{25963}{26970}$	$\frac{7 \cdot 3709}{2 \cdot 3 \cdot 5 \cdot 29 \cdot 31}$	0.962662

TABLE III: Two-Quarterbit ( $\alpha = 2$ ) Separability Probabilities

$k = 0$	$\frac{26}{323}$	$\frac{2 \cdot 13}{17 \cdot 19}$	0.080495
$k = 1$	$\frac{3736}{22287}$	$\frac{2^3 \cdot 467}{3 \cdot 17 \cdot 19 \cdot 23}$	0.167631
$k = 2$	$\frac{1807}{6555}$	$\frac{13 \cdot 139}{3 \cdot 5 \cdot 19 \cdot 23}$	0.275667
$k = 3$	$\frac{3919}{10005}$	$\frac{3919}{3 \cdot 5 \cdot 23 \cdot 29}$	0.391704
$k = 4$	$\frac{104379}{206770}$	$\frac{3 \cdot 11 \cdot 3163}{2 \cdot 5 \cdot 23 \cdot 29 \cdot 31}$	0.504807
$k = 5$	$\frac{16387}{26970}$	$\frac{7 \cdot 2341}{2 \cdot 3 \cdot 5 \cdot 29 \cdot 31}$	0.607601
$k = 6$	$\frac{69475}{99789}$	$\frac{5^2 \cdot 7 \cdot 397}{3 \cdot 29 \cdot 31 \cdot 37}$	0.696219
$k = 7$	$\frac{203123}{263958}$	$\frac{229 \cdot 887}{2 \cdot 3 \cdot 29 \cdot 37 \cdot 41}$	0.769527
$k = 8$	$\frac{1674746}{2022161}$	$\frac{2 \cdot 837373}{31 \cdot 37 \cdot 41 \cdot 43}$	0.828196

tion to the sequence of length eighteen obtained, plus subsequent simplification procedures, yielded the governing rule

$$P_k^{qubit} = 1 - \frac{3 \cdot 4^{k+3} (2k(k+7) + 25) \Gamma(k + \frac{7}{2}) \Gamma(2k+9)}{\sqrt{\pi} \Gamma(3k+13)}. \quad (2)$$

Here  $P_k^{qubit}$  is the separability probability of the (15-dimensional) standard, complex two-qubit systems endowed with the induced measure  $k = K - 4$ . This formula, thus, successfully reproduces the entries of Table II, as well as the subsequent ones ( $k = 9, \dots, 17$ ) we have approximated to high precision, making use of the 11,401 moments in the Provost Legendre-polynomial-based algorithm. (For  $k = 0$ , formula (2) does, in fact, yield the apparent

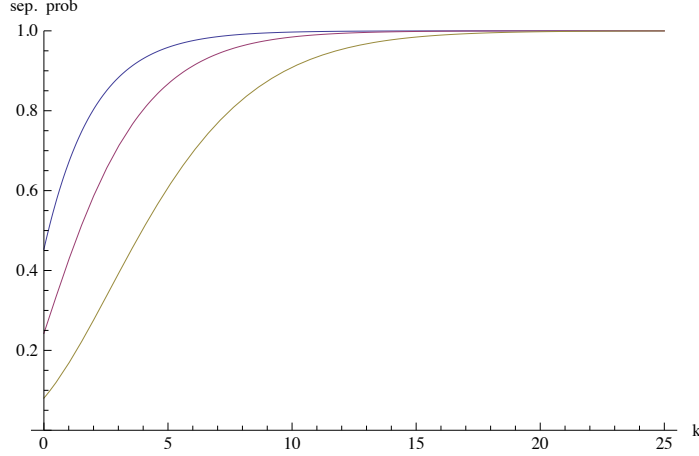


FIG. 1: Two-rebit > two-qubit > two-quaterbit separability probabilities—given by (4), (2) and (3), respectively—as functions of  $k = K - 4$

Hilbert-Schmidt separability probability of  $\frac{8}{33}$  [7–9] [Table II].)

Similarly, employing a somewhat longer sequence  $k = 0, \dots, 21$ , we obtained the quater-nionic ( $\alpha = 2$ ) counterpart

$$P_k^{quaterbit} = 1 - \frac{4^{k+6}(k(k(2k(k+21) + 355) + 1452) + 2430)\Gamma(k + \frac{13}{2})\Gamma(2k + 15)}{3\sqrt{\pi}\Gamma(3k + 22)}, \quad (3)$$

yielding the  $k = 0$  (Hilbert-Schmidt) value of  $\frac{26}{323}$ . Further, for the rebit ( $\alpha = \frac{1}{2}$ ) scenario, making analogous use of the sequence  $k = 0, \dots, 15$ , we found

$$P_k^{rebit} = 1 - \frac{4^{k+1}(8k + 15)\Gamma(k + 2)\Gamma(2k + \frac{9}{2})}{\sqrt{\pi}\Gamma(3k + 7)}, \quad (4)$$

yielding for  $k = 0$ , the result  $\frac{29}{64}$ .

In Fig. 1 we show a joint plot of these three separability probability formulas, with the rebit one ( $\alpha = \frac{1}{2}$ ) dominating the qubit one ( $\alpha = 1$ ), which in turn dominates the quaterbit ( $\alpha = 2$ ) curve. In the limit  $k \rightarrow \infty$ , the three curves/probabilities all approach 1 (cf. [2]). We have found [15, sec. III]—through analytic means—that for each of  $\alpha = 1, 2, 3, 4$  and  $\frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \frac{7}{2}$ , that as  $k \rightarrow \infty$ , the ratio of the logarithm of the  $(k + 1)$ -st separability probability to the logarithm of the  $k$ -th separability probability is  $\frac{16}{27}$ . (Presumably, the pattern continues for larger  $\alpha$ , but the required computations have, so far, proved too challenging.)

It is interesting to observe, additionally, that for  $k = -1$  (that is,  $K = 3$ ), a value not apparently susceptible to use of the principal  $5F4$ -hypergeometric determinantal moment formula and the density approximation (inverse) procedure of Provost [17], the three basic

formulas yield the (now *smaller* than Hilbert-Schmidt) further simple rational values  $\frac{1}{8}$ ,  $\frac{1}{14}$  and  $\frac{11}{442}$ , for the rebit, qubit and quaterbit cases, respectively (cf. [2, p. 130]). Further, for  $k = -2$  ( $K = 2$ ), the rebit formula has a singularity, the qubit formula yields 0, and the quaterbit one gives  $\frac{1}{429} = \frac{1}{3 \times 11 \times 13} \approx 0.002331$ .

We have been able to formally extend this series of three formulas to other values of  $\alpha$ , as well, including  $\alpha = \frac{3}{2}, \frac{5}{2}, 3, \frac{7}{2}, 4, \frac{9}{2}, 5, 6, \dots, 13$  obtaining similarly structured (increasingly larger) formulas. A major challenge that we are continuing to address is to find a *single master* formula that encompasses these several results, and can itself yield the formula for any specific half-integer or integer value of  $\alpha$  (Appendix I).

#### IV. DIVISION OF SEPARABILITY PROBABILITIES BASED ON DETERMINANTAL INEQUALITIES

We have also begun to investigate related aspects of the geometry of random-induced generalized two-qubit states, making use of a *second* hypergeometric-based determinantal moment formula [18, sec. II]

$$\begin{aligned} \left\langle |\rho|^k (|\rho^{PT}| - |\rho|)^n \right\rangle / \left\langle |\rho|^k \right\rangle &= (-1)^n \frac{(\alpha)_n (\alpha + \frac{1}{2})_n (n + 2k + 2 + 5\alpha)_n}{2^{4n} (k + 3\alpha + \frac{3}{2})_n (2k + 6\alpha + \frac{5}{2})_{2n}} \\ &\times {}_4F_3 \left( \begin{matrix} -\frac{n}{2}, \frac{1-n}{2}, k+1+\alpha, k+1+2\alpha \\ 1-n-\alpha, \frac{1}{2}-n-\alpha, n+2k+2+5\alpha \end{matrix}; 1 \right). \end{aligned}$$

The range of the determinant difference variable  $(|\rho^{PT}| - |\rho|)$  is  $[-\frac{1}{16}, \frac{1}{432}]$ , and we shall approximate the contributions over  $[0, \frac{1}{432}]$  to the total separability probabilities given in Tables I, II and III.

In [18], employing the first 9,451 of these moments (having set  $k$  to zero) in the density approximation procedure of Provost [17], we obtained highly convincing numerical evidence that the basic set of three Hilbert-Schmidt separability probabilities  $(\frac{29}{64}, \frac{8}{33}, \frac{26}{323})$  was evenly (symmetrically) split (that is,  $\frac{29}{128}, \frac{4}{33}, \frac{13}{323}$ ) between the two scenarios  $|\rho^{PT}| > |\rho|$  and  $|\rho| > |\rho^{PT}| > 0$ . Now, with the use of 14,051 such determinantal moments, with  $k = 1$ ,  $\alpha = 1$ , we obtained an approximant equal to eight decimal places to  $\frac{45}{286} = \frac{3^{2.5}}{2 \cdot 11 \cdot 13} \approx 0.157342657$  for the case  $|\rho^{PT}| > |\rho|$ . Employing the total separability probability  $k = 1$  result of  $\frac{61}{143}$  in Table II, we find a complementary (larger) approximant of  $\frac{7}{26} = \frac{7}{2 \cdot 13} \approx 0.269230769$ . So, the symmetry present in the Hilbert-Schmidt case (for example,  $\frac{8}{33} = \frac{4}{33} + \frac{4}{33}$ ) is lost for  $k \neq 0$ .



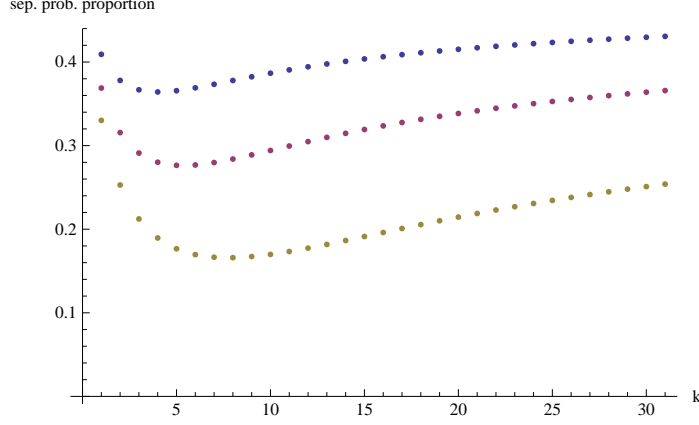


FIG. 2: Proportion of the total random-induced separability probabilities—based on 9,201 moments—accounted for by the region  $|\rho^{PT}| > |\rho|$ . The two-rebit ( $\alpha = \frac{1}{2}$ ) curve is dominant, the two-qubit ( $\alpha = 1$ ), intermediate, and the two-quaterbit ( $\alpha = 2$ ) curve, subordinate.

Similarly, for the  $k = 1$ ,  $\alpha = 2$  counterpart, we obtain an approximant equal, to almost twelve decimal places, to  $\frac{2056}{37145} = \frac{2^3 \cdot 257}{5 \cdot 17 \cdot 19 \cdot 23} \approx 0.0553506528470$ , when  $|\rho^{PT}| > |\rho|$ , and, thus,  $\frac{32}{285} = \frac{2^5}{3 \cdot 5 \cdot 19} \approx 0.1122807017544$  for the complementary (larger) approximant.

To complete the basic triad, that is  $k = 1$  and  $\alpha = \frac{1}{2}$  (for which, convergence is typically weakest), for  $|\rho^{PT}| > |\rho|$ , we have an approximant equal, to more than six decimal places, to  $\frac{281}{1024} = \frac{281}{2^{10}} \approx 0.2744140625$ , and a complementary (larger, again) approximant of  $\frac{1217}{3072} = \frac{1217}{2^{10} \cdot 3} \approx 0.3961588542$ . (Note, again, the occurrence of powers of 2 in the  $\alpha = \frac{1}{2}$  case.)

For  $k = -1$ ,  $\alpha = 2$  it is interesting to note that the approximation of the probability  $|\rho^{PT}| > |\rho|$  is  $\frac{11}{442}$  to ten decimal places. This is the *same* rational value we found above for the *total* separability probability. It, thus, appears that we can conclude that the complementary probability (that is, for  $|\rho| > |\rho^{PT}| > 0$ ) is now *smaller*, in fact, zero, in contrast to the  $k = 1$  case. The complementary probability also appears to be zero for the two companion cases of  $k = -1$ ,  $\alpha = 1$  and  $\alpha = \frac{1}{2}$ .

In Figure 2, we show—based on numerical results using 9,201 moments—the proportion of the three basic total random induced separability probabilities (Tables I, II, III), as a function of  $k$ , accounted for by the region  $|\rho^{PT}| > |\rho|$ . We have been investigating the possibility of obtaining explicit formulas—as we have been able to do above ((2),(3),(4)) for the total separability probabilities (that is, independently of whether  $|\rho| > |\rho^{PT}| > 0$  or  $|\rho^{PT}| > |\rho|$ )—for these sets of complementary probabilities. To even hope to achieve such a

goal, it seems necessary to fill in considerably more rows of Table IV than we have so far been able to do (cf. [15]).

## V. ALTERNATIVE DENSITY APPROXIMATION PROCEDURE

In pursuit of such a goal, we have developed an alternative (Appendix II) to the Legendre-polynomial-based density approximation procedure of Provost [17], which we have made abundant use of above and in our earlier work [7, 8, 18]. Though well-conditioned, it perhaps is relatively slow to converge for our purposes, since it takes as the baseline (starting) distribution, the uniform one, which is far from the sharply-peaked ones, with vanishing endpoints, we have encountered in our separability probability investigations. The approach outlined in Appendix II uses base functions of the form  $((x - a)(b - x))^\alpha$  where  $\alpha$  is a small positive integer. (Provost does present a number of codes, other than the Legendre-polynomial one, including one based on Jacobi polynomials [17, pp. 15, 24]. It employs an adaptive strategy of matching the first and second given moments to those of a beta distribution. But we have found this algorithm to be highly ill-conditioned in our specific applications.)

## VI. CONCLUSIONS

We have reported above some considerable successes in our effort to extend to random induced measures [5, 6], earlier separability probability work [7, 8] based on the Hilbert-Schmidt measure (the particular symmetric  $N = K$  case of the random induced measures), and the inequality  $|\rho^{PT}| > 0$ . Further efforts using the more restrictive inequality  $|\rho^{PT}| > |\rho|$  utilized in sec. IV have been given in a subsequent paper [15]. There equivalences between certain hypergeometric-based formulas and difference equations have been noted.

Let us importantly note that in the recent study [19] the (random induced measure) separability probability problems posed above, have, in fact, been exhaustively *formally* solved for the “toy” seven-dimensional  $X$ -states model [20] of  $4 \times 4$  density matrices. Here, contrastingly, we have concentrated on the more general cases of  $4 \times 4$  density matrices with none of the off-diagonal entries *a priori* nullified (as they are in the  $X$ -states model). Although, we have developed certain formulas here, for which the evidentiary support is

TABLE IV: Proportions of total separability probabilities  $|\rho^{PT}| > |\rho|$

$\alpha$	$\frac{1}{2}$	1	2
$k = 0$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$
$k = 1$	$\frac{843}{2060}$	$\frac{45}{122}$	$\frac{771}{2335}$
$k = 2$	$\frac{9949}{26320}$	$\frac{1553}{4921}$	$\frac{26503}{104806}$
$k = 3$	—	$\frac{3073}{10557}$	$\frac{51585}{242978}$
$k = 4$	—	$\frac{2087}{7450}$	$\frac{2195945}{11586069}$
$k = 5$	—	—	$\frac{4390079}{24859079}$
$k = 6$	—	—	$\frac{8310451}{48993770}$

quite considerable, we still lack formal proofs in this higher-dimensional venue.

We continue to investigate these problems in search of a still more definitive (“master formula”) resolution of them (Appendix I). As a possible tool in such research, we have developed (Appendix II) an alternative density approximation procedure to that of Provost [17], on which we have strongly relied to this point in obtaining exact separability probability results.

## VII. APPENDIX I. MASTER FORMULA INVESTIGATION

This appendix is based on the random induced measure separability probability formulas we have obtained for  $\alpha = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \frac{7}{2}, 1, \dots, 13$ .

The purpose is to find  $P\{|\rho^{PT}| > 0\}$  with respect to the normalized measure  $|\rho|^k$  with parameter  $\alpha$ . The values  $\alpha = \frac{1}{2}, 1, 2$  correspond to the real, complex, quaternion cases respectively. The obtained formulas have the form

$$P\{|\rho^{PT}| > 0\} = 1 - F(\alpha, k).$$

Define

$$G(\alpha, k) := 4^k \frac{\Gamma(k + 3\alpha + \frac{3}{2}) \Gamma(2k + 5\alpha + 2)}{\Gamma(\frac{1}{2}) \Gamma(3k + 10\alpha + 2)}.$$

The first observation: when  $\alpha$  is integer or half-integer  $\frac{F(\alpha, k)}{G(\alpha, k)}$  is a rational function of  $k$ , that is, a ratio of polynomials.

The second observation: when  $\alpha$  is an integer then

$$F(\alpha, k) = p_\alpha(k) G(\alpha, k),$$

where  $p_\alpha(k)$  is a polynomial of degree  $4\alpha - 2$  with leading coefficient  $\frac{2^{8\alpha+1}}{(2\alpha-1)!}$ , and  $p_\alpha$  can be factored as  $(k + g_1(\alpha))(k + g_1(\alpha) + 1) \cdots (k + g_2(\alpha)) \tilde{p}_\alpha(k)$ , where  $\tilde{p}_\alpha(k)$  is irreducible in general; furthermore

$$g_1(\alpha) := 2\alpha + 1 + \left\lfloor \frac{\alpha + 1}{2} \right\rfloor,$$

$$g_2(\alpha) := 3\alpha + \left\lfloor \frac{\alpha + 1}{3} \right\rfloor.$$

The sequence of values  $[g_1(\alpha), g_2(\alpha)]$  for  $\alpha = 2, \dots, 14$  is

$$[6, 7], [9, 10], [11, 13], [14, 17], [16, 20], [19, 23], [21, 27], [24, 30], [26, 33], [29, 37],$$

$$[31, 40], [34, 43], [36, 47]$$

These conjectures imply that the degree of  $\tilde{p}_\alpha(k)$  is

$$4\alpha - 2 - (g_2(\alpha) + 1 - g_1(\alpha)) = 3\alpha + \left\lfloor \frac{\alpha + 1}{2} \right\rfloor - \left\lfloor \frac{\alpha + 1}{3} \right\rfloor - 2.$$

The coefficient of  $k^{4\alpha-3}$  in  $\left(\frac{2^{8\alpha+1}}{(2\alpha-1)!}\right)^{-1} p_\alpha(k)$  (note that this is monic, coefficient of  $k^{4\alpha-2}$  is 1) is given by

$$c_2(\alpha) := -3 + \frac{3}{2}\alpha + \frac{17}{2}\alpha^2 + \left(\left\lfloor \frac{\alpha - 1}{4} \right\rfloor - \left\lfloor \frac{\alpha}{4} \right\rfloor\right) \left(1 + \frac{5}{2}\alpha\right),$$

equivalently

$$c_2(\alpha) = \begin{cases} -4 - \alpha + \frac{17}{2}\alpha^2, & \alpha \equiv 0 \pmod{4}, \\ -3 + \frac{3}{2}\alpha + \frac{17}{2}\alpha^2, & \alpha \not\equiv 0 \pmod{4}. \end{cases}$$

To determine the second coefficient of  $\tilde{p}_\alpha$  note that the second coefficient of  $(k^n + a_2 k^{n-1} + \dots)(k^m + b_2 k^{m-1} + \dots) = k^{n+m} + (a_2 + b_2)k^{n+m-1} + \dots$  is  $a_2 + b_2$ , so the second coefficient of  $(k + g_1(\alpha))(k + g_1(\alpha) + 1) \cdots (k + g_2(\alpha))$  is subtracted from  $c_2(\alpha)$ . This coefficient is

$$c'_2(\alpha) := \sum_{i=g_1(\alpha)}^{g_2(\alpha)} i = \frac{1}{2} (g_1(\alpha) + g_2(\alpha)) (g_2(\alpha) - g_1(\alpha) + 1)$$

$$= \frac{1}{2} \left( 5\alpha + 1 + \left\lfloor \frac{\alpha + 1}{2} \right\rfloor + \left\lfloor \frac{\alpha + 1}{3} \right\rfloor \right) \left( \alpha + \left\lfloor \frac{\alpha + 1}{3} \right\rfloor - \left\lfloor \frac{\alpha + 1}{2} \right\rfloor \right).$$

The second coefficient of  $\tilde{p}_\alpha$  is  $c_2(\alpha) - c'_2(\alpha)$ ; the sequence of values for  $\alpha = 1 \dots 14$  is

$$[7, 21, 59, 92, 155, 222, 319, 364, 510, 626, 745, 853, 1068, 1186].$$

Denote the coefficient of  $k^{4\alpha-4}$  in  $\left(\frac{2^{8\alpha+1}}{(2\alpha-1)!}\right)^{-1} p_\alpha(k)$  by  $c_3(\alpha)$  then from the calculated values ( $\alpha = 1, \dots, 13$ ) we find for  $\alpha \neq 0 \bmod 4$  that

$$c_3(\alpha) = 11 - \frac{389}{24}\alpha - \frac{333}{16}\alpha^2 + \frac{115}{48}\alpha^3 + \frac{289}{8}\alpha^4.$$

The third observation: when  $\alpha$  is a half-integer then

$$F(\alpha, k) = \frac{p_\alpha(k)}{(k + 2\alpha + 1)_{\alpha+1/2}} G(\alpha, k),$$

where  $p_\alpha(k)$  is a polynomial of degree  $5\alpha - \frac{3}{2}$  with leading coefficient  $\frac{2^{8\alpha+1}}{(2\alpha-1)!}$ .

## VIII. APPENDIX II. A MODIFICATION OF THE PROVOST-LEGENDRE METHOD USING GEGENBAUER POLYNOMIALS

We consider the problem of approximating a density function with given moments using Jacobi polynomials for some choice of parameters. The technique uses a construction of Provost [17, sec. 4] which is adapted for a specific aspect of the unknown probability density, namely,  $\Pr\{X > 0\}$ .

Suppose the density  $f(x)$  is supported on the interval  $[a, b]$  with given (i.e. computable) moments  $\mu_n := \int_a^b x^n f(x) dx$ , and  $\{p_n(x)\}$  is a family of orthogonal polynomials with weight function  $w(x)$  also on  $[a, b]$ ; the structure constants are

$$h_n := \int_a^b p_n(x)^2 w(x) dx, \quad n = 0, 1, 2, \dots$$

The aim is to (implicitly) determine the expansion

$$f(x) = \sum_{n=0}^{\infty} \lambda_n p_n(x) w(x).$$

and to apply it to the approximation of (where  $a < 0 < b$ )

$$\Pr\{X > 0\} = \int_0^b f(x) dx = \sum_{n=0}^{\infty} \lambda_n \int_0^b p_n(x) w(x) dx.$$

By orthogonality, for  $m = 0, 1, 2, \dots$

$$\begin{aligned} \int_a^b p_m(x) f(x) dx &= \sum_{n=0}^{\infty} \lambda_n \int_a^b p_n(x) p_m(x) w(x) dx \\ &= \lambda_m h_m. \end{aligned}$$

To evaluate the left hand side compute the coefficients  $\{a_{ni} : 0 \leq i \leq n\}$  in the expansions

$$p_n(x) = \sum_{i=0}^n a_{ni} x^i,$$

when  $\{p_n(x)\}$  are shifted Jacobi polynomials (this requires extra computation since the shortest expansions are in powers of  $(x - a)$  or  $(b - x)$ ); then

$$\begin{aligned} \lambda_m h_m &= \int_a^b \sum_{i=0}^m a_{mi} x^i f(x) dx = \sum_{i=0}^m a_{mi} \mu_i, \\ \lambda_m &= \frac{1}{h_m} \sum_{i=0}^m a_{mi} \mu_i; \end{aligned}$$

The main problem is to approximate  $\int_{\xi}^b f(x) dx$  for some given  $\xi$ : so

$$\int_a^{\xi} f(x) dx = \sum_{n=0}^{\infty} \lambda_n \int_{\xi}^b p_n(x) w(x) dx.$$

Compute

$$q_n := \int_{\xi}^b p_n(x) w(x) dx,$$

then

$$\begin{aligned} \int_{\xi}^b f(x) dx &= \sum_{n=0}^{\infty} \lambda_n q_n = \sum_{n=0}^{\infty} \frac{1}{h_n} \sum_{i=0}^n a_{ni} \mu_i q_n \\ &= \sum_{i=0}^{\infty} \mu_i \sum_{n=i}^{\infty} \frac{q_n}{h_n} a_{ni}, \end{aligned}$$

and now we observe that the sum over  $n$  is the coefficient of  $x^i$  in

$$\sum_{n=0}^{\infty} \frac{q_n}{h_n} p_n(x).$$

Truncate the infinite series to obtain an approximation.

**Jacobi polynomials:** We start with background information about general parameters and then specialize to equal parameters. The family  $\{P_n^{(\alpha, \beta)}(t)\}$  is orthogonal for

$$(1-t)^\alpha (1+t)^\beta;$$

$$\begin{aligned} P_n^{(\alpha,\beta)}(t) &= \frac{(\alpha+1)_n}{n!} {}_2F_1\left(\begin{matrix} -n, n+\alpha+\beta+1 \\ \alpha+1 \end{matrix}; \frac{1-t}{2}\right) \\ \frac{d}{dt} \left\{ (1-t)^{\alpha+1} (1+t)^{\beta+1} P_{n-1}^{(\alpha+1,\beta+1)}(t) \right\} &= -2n (1-t)^\alpha (1+t)^\beta P_n^{(\alpha,\beta)}(t) \\ h_n &= 2^{\alpha+\beta+1} B(\alpha+1, \beta+1) \frac{(\alpha+1)_n (\beta+1)_n (\alpha+\beta+n+1)}{n! (\alpha+\beta+2)_n (\alpha+\beta+2n+1)}. \end{aligned} \quad (5)$$

Equation (5) is from [21, 18.9.16]. To shift to the interval  $[a, b]$  set

$$\begin{aligned} x &= \frac{1}{2} ((b-a)t + a + b), \quad t = \frac{2x - a - b}{b - a} \\ w(x) &= \left(\frac{2}{b-a}\right)^{\alpha+\beta+1} (b-x)^\alpha (x-a)^\beta, \\ p_n(x) &= P_n^{(\alpha,\beta)}\left(\frac{2x - a - b}{b - a}\right), \end{aligned}$$

and the key quantities  $q_n$  are found by

$$\begin{aligned} \int_\xi^b p_n(x) w(x) dx &= \left(\frac{2}{b-a}\right)^{\alpha+\beta+1} \int_\xi^b P_n^{(\alpha,\beta)}\left(\frac{2x - a - b}{b - a}\right) (b-x)^\alpha (x-a)^\beta dx \\ &= \int_\zeta^1 P_n^{(\alpha,\beta)}(t) (1-t)^\alpha (1+t)^\beta dt \\ &= -\frac{1}{2n} \int_\zeta^1 \frac{d}{dt} \left\{ (1-t)^{\alpha+1} (1+t)^{\beta+1} P_{n-1}^{(\alpha+1,\beta+1)}(t) \right\} dt \\ &= \frac{1}{2n} (1-\zeta)^{\alpha+1} (1+\zeta)^{\beta+1} P_{n-1}^{(\alpha+1,\beta+1)}(\zeta), \quad n \geq 1; \\ \zeta &= \frac{2\xi - a - b}{b - a}, \end{aligned}$$

and  $q_0 = \int_\zeta^1 (1-t)^\alpha (1+t)^\beta dt$ .

In the case  $a = -\frac{1}{16}, b = \frac{1}{432}, \xi = 0$  the transformations are

$$\begin{aligned} t &= \frac{216}{7}x + \frac{13}{14}, \quad \zeta = \frac{13}{14}, \\ p_n(x) &= P_n^{(\alpha,\beta)}\left(\frac{216}{7}x + \frac{13}{14}\right). \end{aligned}$$

Thus the strategy is to choose appropriate parameters  $\alpha, \beta$  (small integer values appear to work well), then determine the coefficients of  $\{x^i\}$  in the truncated series

$$\sum_{n=0}^{\infty} \frac{q_n}{h_n} P_n^{(\alpha,\beta)}\left(\frac{2x - a - b}{b - a}\right).$$

**Computational details:**

Given  $[a, b]$  with  $a < 0 < b$  let  $c_0 := -\frac{a+b}{b-a}$ ,  $c_1 := \frac{2}{b-a}$  and specialize to  $\alpha = \beta = \lambda - \frac{1}{2} \geq 0$ , so that the weight is  $(1-t^2)^\alpha$  and the Gegenbauer polynomials  $P_n^\lambda$  form the orthogonal basis. We use the normalized polynomials with  $P_n^\lambda(1) = 1$ . (Note that  $P_n^\lambda(t) = \frac{n!}{(\lambda + \frac{1}{2})_n} P_n^{(\lambda-1/2, \lambda-1/2)}(t)$ .) The recurrence is  $P_0^\lambda(t) = 1, P_1^\lambda(t) = t$ ,

$$P_{n+1}^\lambda(t) = \frac{2n+2\alpha+1}{n+2\alpha+1} t P_n^\lambda(t) - \frac{n}{n+2\alpha+1} P_{n-1}^\lambda(t), n \geq 1$$

and

$$h_n = \frac{\Gamma(\frac{1}{2}) \Gamma(\alpha+1)}{\Gamma(\alpha + \frac{3}{2})} \frac{n! (2\alpha+1)}{(2\alpha+1)_n (2n+2\alpha+1)} = h_0 \eta_n,$$

where

$$\eta_0 = 1, \eta_n = \frac{n(2n+2\alpha-1)}{(2n+2\alpha+1)(n+2\alpha)} \eta_{n-1}, n \geq 1.$$

(see [22, Sect. 1.4.3]). In the recurrence replace  $t$  by  $c_0 + y$ , where  $y = c_1 x$  (this takes the scaling factor out of the computations) Let

$$P_n^\lambda(c_0 + y) = \sum_{j=0}^n B_{nj} y^j,$$

then (with the convention  $B_{n,-1} = 0$ )

$$\begin{aligned} B_{00} &= 1, B_{1,0} = c_0, B_{1,1} = 1, \\ B_{nj} &= \frac{2n+2\alpha-1}{n+2\alpha} (c_0 B_{n-1,j} + B_{n-1,j-1}) - \frac{n-1}{n+2\alpha} B_{n-2,j}, n \geq 2, 0 \leq j \leq n. \end{aligned}$$

Furthermore

$$\begin{aligned} \frac{d}{dt} \left\{ (1-t^2)^{\alpha+1} P_{n-1}^{\lambda+1}(t) \right\} &= -2(\alpha+1) (1-t^2)^\alpha P_n^\lambda(t), \\ q_n &= \int_{c_0}^1 (1-t^2)^\alpha P_n^\lambda(t) dt = \frac{1}{2(\alpha+1)} (1-c_0^2)^{\alpha+1} P_{n-1}^{\lambda+1}(c_0), n \geq 1, \\ q_0 &= \int_{c_0}^1 (1-t^2)^\alpha dt, \end{aligned}$$

and  $P_{n-1}^{\lambda+1}(c_0) = g_n$  can be computed with the recurrence

$$\begin{aligned} g_1 &= 1, g_2 = c_0, \\ g_n &= \frac{2n+2\alpha-1}{n+2\alpha+1} c_0 g_{n-1} - \frac{n-2}{n+2\alpha+1} g_{n-2}, \end{aligned}$$

thus  $q_1 = \frac{1}{2(\alpha+1)} (1-c_0^2)^{\alpha+1}$  and  $q_n = g_n q_1$ . Note: if  $\alpha$  and  $c_0$  are rational then the quantities  $\{B_{nj}\}$ ,  $\{\eta_n\}$  and  $\{g_n\}$  can be computed in exact arithmetic.



Suppose the process is terminated at some  $m$ , then (approximate values)

$$A_0 = \frac{q_0}{h_0} + \frac{q_1}{h_0} \sum_{j=1}^m \frac{g_j}{\eta_j} B_{j,0}$$

$$A_i = c_1^i \frac{q_1}{h_0} \sum_{j=i}^m \frac{g_j}{\eta_j} B_{j,i}, \quad 1 \leq i \leq m.$$

Since polynomial interpolation tends to be not numerically well-conditioned (a lot of cancellation) it is suggested to compute the quantities  $\{q_j\}, \{B_{j,i}\}$  to high precision, or even better, in exact arithmetic for  $\alpha = 0, 1, 2, \dots$

### Conflict of Interests

The authors declare that there is no conflict of interests regarding the publication of this paper.

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- [1] K. Życzkowski, P. Horodecki, A. Sanpera, and M. Lewenstein, Phys. Rev. A **58**, 883 (1998).
  - [2] G. Aubrun, S. J. Szarek, and D. Ye, Commun. Pure Appl. Math. **LXVII**, 0129 (2014).
  - [3] U. T. Bhosale, S. Tomsovic, and A. Lakshminarayan, Phys. Rev. A **85**, 062331 (2012).
  - [4] R. Singh, R. Kunjwal, and R. Simon, Phys. Rev. A **89**, 022308 (2014).
  - [5] K. Życzkowski and H.-J. Sommers, J. Phys. A **A34**, 7111 (2001).
  - [6] I. Bengtsson and K. Życzkowski, *Geometry of Quantum States* (Cambridge, Cambridge, 2006).
  - [7] P. B. Slater and C. F. Dunkl, J. Phys. A **45**, 095305 (2012).
  - [8] P. B. Slater, J. Phys. A **46**, 445302 (2013).
  - [9] J. Fei and R. Joynt, arXiv.1409:1993.
  - [10] S. Milz and W. T. Strunz, J. Phys. A **48**, 035306 (2015).
  - [11] A. Khvedelidze and I. Rogojina (2013), Joint Institute for Nuclear Research, Dubna.
  - [12] A. Peres, Phys. Rev. Lett. **77**, 1413 (1996).
  - [13] K. Życzkowski and H.-J. Sommers, J. Phys. A **36**, 10115 (2003).

- [14] I. Dumitriu and A. Edelman, J. Math. Phys. **43**, 5830 (2002).
- [15] P. B. Slater, arXiv:1504.04555.
- [16] M. Horodecki, P. Horodecki, and R. Horodecki, Phys. Lett. A **223**, 1 (1996).
- [17] S. B. Provost, Mathematica J. **9**, 727 (2005).
- [18] P. B. Slater and C. F. Dunkl, J. Geom. Phys. **90**, 42 (2015).
- [19] C. F. Dunkl and P. B. Slater, arXiv:1501.02289.
- [20] P. Mendonça, M. A. Marchioli, and D. Galetti, Anns. Phys. **351**, 79 (2014).
- [21] F. Olver, D. Lozier, R. Boisvert, and C. Clark, *NIST Handbook of Mathematical Functions* (Cambridge Univ. Press, Cambridge, 2010).
- [22] C. Dunkl and Y. Xu, *Orthogonal Polynomials of Several Variables* (Cambridge Univ. Press, Cambridge, 2014).